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A SIMPLE REACTION-RATE MODEL FOR TURBULENT DIFFUSION FLAMES

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Abstract

A simple reaction-rate model is proposed for turbulent diffusion flames. This model was derived from the results of Chung (1972), and has reaction rate proportional to turbulence mixing rate. The reaction rate is also dependent on the mean mass fraction and the mean-square fluctuation of mass fraction of each reactant. Calculations are compared with experimental data of Kent and Bilger(1973), and are generally successful in predicting the measured quantities.

Nomenc:Lature

a, b, đ	Stoichiometric coefficients of fuel, oxygen, and product, respectively
c _i	mass fraction of specie i; c, turbulent fluctuation
c _{€1} , c _{€2}	empirical constar 3, equal to 1.43 and 1.92, respectively
c _{g1} , c _{g2}	empirical constants, equal to 3.0 and 0.20, respectively
c _µ	empirical constant, equal to 0.09
ת	diameter of hydrogen injector
gi	mean-square fluctuation of mass fraction, c_i^2
h	static enthalpy
Ł _o	stagnation enthalpy
k	mean turbulence kinetic energy, uui/2
p	pressure
r	radial distance from the axis of symmetry
U, V	velocity in x, y directions
u, v	turbulence velocity in x, y directions

<u>u</u>. jet mass-average velocity ₩. molecular weight of specie i $\mathbf{\mathring{w}_{i}}$ reaction rate of specie i Cartesian coordinates x, y dissipation rate of turbulence eddy viscosity μ_{T} density ρ turbulent Prandtl-Schmidt number for transport of quantity j; $\sigma_f = \sigma_g = \sigma_h = \sigma_{\bar{\Phi}} = 0.7; \quad \sigma_k = 1.0; \quad \sigma_{\bar{e}} = 1.3$ ()mean or time-average value of ()

Subscripts

- c centerline value
- e free-stream conditions outside mixing region
- f fuel
- J fuel jet at injection location
- N nitrogen
- o oxygen

Introduction

There have been a number of studies directed toward modeling the effect of turbulence on chemical reactions. These studies have been motivated by the need to develop methods for computing turbulent, chemically-reacting flow fields for a wide variety of applications. Spalding proposed three such models 1-3, all for cases where the chemical reaction time is much less than the characteristic time for turbulent mixing. His first model was for

initially unmixed reactants that react instantly on contact. It was assumed that the instantaneous fuel-air ratio at a point was equal to the mean value, plus or minus the root-mean-square fluctuation. For each of these two values, the temperature and composition for complete reaction was computed.

Calculations indicated a finite flame width, which is qualitatively correct.

This model has not been extensively compared with experiment, however. Spalding's second and third models^{2,3} were developed for premixed flames, and were called eddy breakup models. Each had the mean fuel reaction rate proportional to •/k, the characteristic mixing rate of the turbulence. The second and third models also had mean fuel reaction rate proportional to mean fuel mass fraction and to root-mean-square fluctuation of fuel mass fraction, respectively. Both of these models have had some success when compared with experimental data for premixed flows.

Rhodes, Harsha and Peters did not use species conservation equations, and so did not model the reaction-rate terms directly. They divided the flow field into classes and zones, characterized by instantaneous and mean concentrations of the fuel, respectively. An assumed probability density for concentration fluctuations was used to develop a model for their effect on mean density. (Correlations involving density fluctuations were neglected, however). This model was combined with both equilibrium chemistry and finite-rate chemistry models. In the latter, each class was assumed to behave as a one-dimensional, transient stirred reactor. Their computations were compared with the data of Kent and Bilger for $\tilde{U}_{1}/\tilde{U}_{p}=10$.

Hilst, et al⁶, developed second-order closure methods for the species continuity equations, and combined these with turbulent diffusion models.

These models conformed to the principles of invariant modeling. A limited number of calculations were performed for two-dimensional diffusion and isothermal reaction of two species. Libby considered the equations

describing turbulent reacting flows with fast chemical reactions. Effects of density fluctuations were included in the formulation. Specific closure models were not proposed, however.

There have also been a number of studies which considered simplified flow fields, in an effort to describe the interaction between turbulence and chemical reactions in greater detail. Among these are Chung⁸, Alber and Batt⁹, and O'Brien^{10,11}. In these analyses, the probability density functions for velocity and scalar fluctuations were modeled and used to compute various correlations. The analysis of Chung⁸ formed the basis of the model described here.

This paper has two purposes. First to propose a simple reaction-rate model applicable to turbulent diffusion flames, for which the time scale for chemical reaction is much smaller than the time scale for turbulent mixing. Second, to provide a limited assessment of the proposed model by comparing calculations with experimental data.

Reaction-Rate Model

In this section, Chung's analysis of homologous shear flow forms the basis for a model of the chemical reaction rate in a turbulent flow. It is assumed that the chemical reaction time is much less than the turbulent mixing time. Also, it is assumed that the Reynolds number is large and that solid boundaries have negligible influence, so that molecular transport can be neglected.

Chung considered a one-dimensional shear flow with nonzero derivatives in the y-direction, only. He also assumed constant density, so that the velocity field was not affected by the temperature field. For these conditions,

the mean species conservation equation for the fuel (f) is:

$$\frac{\mathrm{d}}{\mathrm{d}\mathbf{y}} \left(\nabla \mathbf{c}_{\mathbf{f}} \right) = \mathbf{v}_{\mathbf{f}} \tag{1}$$

In his solution, Chung represented the probability density of the fluid elements by the sum of two half-Maxwellian functions containing a total of four parameters. A moment method was used to solve for these parameters. These in turn determined mean velocity gradient, turbulence energy, and Reynolds stress.

Next, consider that the combustion is described by the following onestep chemical reaction:

a (fuel) + b (oridizer)
$$\rightarrow$$
 d (product) (2)

Chung's solution for the probability densities, when the chemical reaction time is much smaller than the turbulent mixing time, allows the correlation vc, to be evaluated. It is:

$$\overline{vc_f} = \left[(1 - \pi/8) k/3\pi \right]^{0.5} c_f$$
 (3)

In the combustion region, the solution for $C_{\mathbf{f}}$ is linear in y. Although Chung did not explicitly do so, an equation for $\mathbf{w}_{\mathbf{f}}$ can be obtained by substituting (3) and the solution for $C_{\mathbf{f}}$ into (1) After some manipulation, the result can be expressed as:

$$\overline{\hat{\mathbf{w}}_{\mathbf{f}}} = - (3/8\pi) \ 2^{0.5} \ (\mathbf{k}^{0.5}/\ell) \left[\overline{\mathbf{c}}_{\mathbf{f}} + \mathbf{g}_{\mathbf{f}}^{0.5} + (\mathbf{w}_{\mathbf{f}} \mathbf{e}/\mathbf{w}_{\mathbf{o}} \mathbf{b}) \ (\overline{\mathbf{c}}_{\mathbf{o}} + \mathbf{g}_{\mathbf{o}}^{0.5}) \right]$$
(4)

where ℓ is the local integral scale of the turbulence. In (4), the rate

 $k^{0.5}/\ell$ is consistent with the condition that turbulent motion controls the reaction rate. The quantity in brackets provides an estimate of the effect of the amount of each reactant on the reaction rate.

It is here hypothesized that (4) is approximately valid at each point in more complex flows than the one-dimensional shear flow considered by Chung⁸. This hypothesis was incorporated into a calculation method that uses differential equations for k and ε to describe turbulence transport¹². If the estimate $\varepsilon = k^{1.5}/\ell$ is made ¹⁴, (4) can be written in terms of k and ε as:

$$\frac{1}{\tilde{w}_{p}} = -A(\epsilon/k) \left[\tilde{c}_{p} + g_{p}^{O.5} + (\tilde{w}_{p}a/\tilde{w}_{o}b)(\tilde{c}_{o} + g_{o}^{O.5}) \right]$$
 (5)

where A is about 0.17. Comparisons with experimental data, to be discussed in the next section, suggest that A = 0.22 is a better estimate.

The dependence of $\overline{w_f}$ on mass fraction resembles a result derived by Gibson and Libby 15 for steady flow relative to a reaction zone, with oxidizer and product on one side and fuel and product on the other. Their solution has $C_f(-\infty)$ instead of $\overline{C_f} + g_f^{0.5}$, and $C_o(\infty)$ instead of $\overline{C_o} + g_o^{0.5}$. Here $C_f(-\infty)$ and $C_o(\infty)$ are the mass fractions of fuel and oxidizer in the volumes adjacent to the reaction zone. Following Gibson and Libby 15, (5) may perhaps be interpreted as a mean rate of consumption of fuel at a point, related to the frequency of passage of reaction zones through that point. Equation (5) is also related to Spalding's models for premixed flames, in that $\overline{w_f}$ is proportional to e/k. The dependence on amount of reactants is different, however. It is evident that $\overline{w_f}$ as calculated by (5) does not go to zero when one of the reactants disappears. For this reason $\overline{w_f}$ was set equal to zero when the sum of the mean value and the root-mean-square fluctuation of

mass fraction of either reactant was less than 10-4.

The differential equations for g_f and g_o also contain reaction rate terms, $c_f \rho w_f$ and $c_o \rho w_o$, respectively. For the one-dimensional shear flow studied by Chung⁸, the species conservation equation for fuel can be written, after multiplying by C_ρ and taking the time average, as:

$$\frac{d}{dv} \left(v c_f^2 / 2 \right) = \overline{c_f \dot{w_f}} \tag{6}$$

Using Chung's solution for the probability densities to evaluate vor gives:

$$\overline{C_f w_f} = (\overline{C_f} + g_f^{0.5}) \overline{w_f}$$

so that $c_f \stackrel{\circ}{w_f} = g_f^{0.5} \stackrel{\circ}{w_f}$. This can be used in the equation for g_f by neglecting density fluctuations, giving $c_f \stackrel{\circ}{p} \stackrel{\circ}{w_f} = \stackrel{\circ}{p} g_f^{0.5} \stackrel{\circ}{w_f}$.

Summary of Equations

The folicing is a summary of the mean differential equations that were solved. They are written for axially symmetric flow in the boundary-layer approximation. Density fluctuations have been neglected. Various turbulence transport terms have been modeled as described by Launder and Spalding 12,13. The conservation equations are:

Mass:
$$\partial(\bar{\rho} \, \bar{\mathbf{U}}\mathbf{r})/\partial\mathbf{x} + \partial(\bar{\rho} \, \bar{\mathbf{V}}\mathbf{r})/\partial\mathbf{r} = 0$$
 (7)

x-momentum:
$$\bar{\rho} \ \bar{U} \ \partial \bar{U}/\partial x + \bar{\rho} \ \bar{V} \ \partial \bar{U}/\partial r = r^{-1}(\partial/\partial r)(r\mu_{\eta} \ \partial \bar{U}/\partial r) - d\bar{\rho}/dx$$
 (8)

where

$$\mu_{\rm T} = C_{\mu} \bar{\rho} k^2/\epsilon \tag{9}$$

Energy:
$$\ddot{\rho} \ \ddot{0} \ \partial \ddot{h}_{O} / \partial x + \ddot{\rho} \ \ddot{v} \ \partial \ddot{h}_{O} / \partial r = r^{-1} (\partial/\partial r) \Big[r (\mu_{T} / \sigma_{h}) \partial \ddot{h} / \partial r$$
 (10)
$$+ r \mu_{\eta} \ddot{u} \ \partial \ddot{u} / \partial r \Big]$$

where

$$\bar{h}_{o} = \bar{h} + \frac{1}{2}\bar{v}^2 + k$$

Fuel:
$$\vec{p} \ \vec{v} \ \partial \vec{c}_f / \partial x + \vec{p} \ \vec{v} \ \partial \vec{c}_f / \partial r =$$

$$r^{-1} (\partial / \partial r) \left[r(\mu_T / \sigma_f) \ \partial \vec{c}_f / \partial r \right] + \vec{p} \ \vec{k}_f$$
(11)

Reaction
$$\bar{\rho} \ \bar{U} \ \partial \bar{C} / \bar{v}_{x} + \bar{\rho} \ \bar{V} \ \partial \bar{C} / \partial r = r^{-1} (\partial/\partial r) \left[r(\mu_{T}/\sigma_{\rho}) \partial \bar{C} / \partial r \right]$$
 (12)

w ere

$$\ddot{C}_{\phi} = \ddot{C}_{o} - (W_{o}b/W_{f}a) \ddot{C}_{f}$$

Fuel
$$\vec{p}$$
 \vec{U} $\partial g_{\vec{I}}/\partial x + \vec{p}$ \vec{V} $\partial g_{\vec{I}}/\partial r = r^{-1}(\partial/\partial r) \left[r(\mu_{\vec{I}}/\sigma_{\vec{g}}) \partial g_{\vec{I}}/\partial r \right]$ (13)
 $+ c_{\vec{g} \vec{L}} \mu_{\vec{I}} (\partial \vec{c}_{\vec{I}}/\partial r)^2 - c_{\vec{g} \vec{L}} \vec{p}^2 \times g_{\vec{I}}/\mu_{\vec{I}} + 2 \vec{p} g_{\vec{I}}^{0.5} \vec{w}_{\vec{I}}$

The equation for oxygen fluctuations is the same as (13), but with g_f , \bar{c}_f , and $\overline{\psi}_f$ replaced by g_o , \bar{c}_o , and $\overline{\psi}_o$, respectively. Here, $\overline{\psi}_o$ equals (W_ob/W_fa) $\overline{\psi}_f$.

Turbulence kinetic
$$\bar{\rho} \ \bar{U} \ \partial k / \partial x + \bar{\rho} \ \bar{V} \ \partial k / \partial r = r^{-1} (\partial / \partial r) \left[r (\mu_{\underline{T}} / \sigma_{\underline{k}}) \ \partial k / \partial r \right]$$
 (14)
$$+ \mu_{\underline{T}} (\partial \bar{U} / \partial r)^{2} - \bar{\rho} \epsilon$$

$$\vec{p} \cdot \vec{U} \cdot \partial \varepsilon / \partial x + \vec{p} \cdot \vec{V} \cdot \partial \varepsilon / \partial r = r^{-1} (\partial / \partial r) \left[r(\mu_{T} / \sigma_{\varepsilon}) \cdot \partial \varepsilon / \partial r \right]$$

$$+ c_{\varepsilon 1} (\varepsilon / k) \mu_{T} (\partial \vec{U} / \partial r)^{2} - c_{\varepsilon 2} \cdot \vec{p} \cdot \varepsilon^{2} / k$$
(15)

There is also a differential equation for \bar{c}_N , of the same form as (12). These differential equations were supplemented by equations of state, which assume a mixture of perfect gases with variable specific heats. The numerical solution was performed using a finite-difference method based on that of Patankar and Spalding 16 .

Comparisons with Experiment

A limited evaluation of this reaction-rate model has been made by comparing calculations with the experimental data of Kent and Bilger for velocity ratios \tilde{U}_J/\tilde{U}_e equal to 10, 5, and 2. These experiments were chosen as a standard of comparison because of the extensive flow field measurements, including initial conditions for u^2 . The experimental arrangement was a central hydrogen jet issuing into a parallel, coaxial air stream. Both streams were subsonic and initially at about 300K. There was a slight favorable pressure gradient, caused by the influence of the tunnel walls.

The initial conditions and the pressure gradient for the calculations were the same as those measured. k and were not measured directly, however. The initial values of k were determined by $k \cong \overline{u^2}/4 \, C_{\mu}^{0.5}$, based on conditions in the inertial sublayer of a boundary layer. Initial values of were determined from k and the measured $\overline{u}(y)$ through the approximation $c = c_{\mu}^{0.5} \, k \, d\overline{u}/dr$. This was based on the approximation that

Reynold stress is proportional to k, and on (9). Initial conditions for g_f were assumed to be $g_f = 2k(\bar{c}_f/\bar{c})^2$, and similarly for g_o .

The most extensive set of measurements reported by Kent and Bilger were for $\ddot{U}_{1}/\ddot{U}_{0}=10$. In making calculations for this case, a number of values of the coefficient A in (5) were tried. The value 0.22 gave somewhat better comparison with experiment than the original estimate of 0.17. Figures 1-7 show comparisons of calculations using A = 0.22 with experiments for $\vec{\mathbf{U}}_{_{\mathrm{T}}}/\vec{\mathbf{U}}_{_{\mathrm{S}}} = 10$. Figure 1 shows the axial variation of centerline values of temperature and of mole fraction of H2, O2, and H2O. Figures 2-5 show radial profiles of these four quantities at x/D of 40, 80, 120, and 160. These comparisons show satisfactory agreement overall, and are generally best nearer the injector (smaller x/D) and choser to the centerline (smaller r/r_A). The latter may be related to the omission from the analysis of intermittency effects. Also, the omission of correlations involving density fluctuations is expected to be important at larger $r/r_{\rm J}$, where there are large density gradients. Figures 3 and 5 also show results calculated by Rhodes, et al4, using an integral method, with equilibrium chemistry and their model for the mean density. At x/D = 80 (Figure 3), the present method and that of Rhodes, et al, are both in good agreement with experiment. At x/D = 160 (Figure 5), however, the results of the present method are in substantially better agreement with experiment.

Figure 6 shows flame contours. The H_2 and O_2 limits are where the mole fractions of H_2 and O_2 are 0.01 and 0.005, respectively. The stoichiometric line is where H_2 and O_2 appear in stoichiometric proportions. If the intersection of the stoichiometric line with the axis is used as a measure of flame length, then the calculation overpredicts this case by about

7%. Turbulence levels on the axis are shown in Figure 7. The calculated line is based on the assumption that v^2 equals (2/3) k, as for isotropic turbulence.

Calculations were also made for \bar{U}_J/\bar{U}_e of 5 and 2 using A equal to 0.22. Figure 8 shows the axial variation of temperature and of mole fractions of H_2 , O_2 , and H_2O for $\bar{U}_J/\bar{U}_e=5$. Radial profiles of these quantities at x/D of 40 are shown in Figure 9. The same information for $\bar{U}_J/\bar{U}_e=2$ is shown in Figures 10 and 11. These comparisons show rather close agreement with experiment, as for $\bar{U}_J/\bar{U}_e=10$. This lends some support to the idea that the coefficient A is nearly a constant, although this is not conclusive. Again there is generally better agreement for smaller x/D and smaller r/r_T .

The axial variation of mean velocity for all three velocity ratios is compared with experiment in Figure 12. For \bar{U}_J/\bar{U}_e of 10 and 5, calculations are within about % of experiment. Differences of up to 16% occur for $\bar{U}_J/\bar{U}_e=2$, however. This may be a result of the turbulence transport model, because when the velocity excess in the jet is small, the model predicts a velocity decay rate that is slower than measured 17 . This applies for $\bar{U}_J/\bar{U}_e=2$, where for example at x/D=80, the calculation gave $\bar{U}_c/\bar{U}_e=1.052$.

Although the reaction-rate model proposed here greatly simplifies the actual physical behavior, this model and the turbulence transport model level generally successful in predicting measured values from the experiments of Kent and Bilger. The favorable results obtained so far, plus the ease of use of the model, justify further consideration of this reaction-rate model for turbulent diffusion flame calculations.

Summary

The simple reaction-rate model for turbulent diffusion flames proposed here has the following major characteristics: (1) the reaction rate is proportional to the turbulence mixing rate; (2) the reaction rate is dependent on the mean mass fraction and on the mean square fluctuation of mass fraction of each reactant.

Computations using this reaction-rate model have been generally successful in predicting measured quantities for three hydrogen jet to air stream velocity ratios from the experiments of Kent and Bilger⁵.

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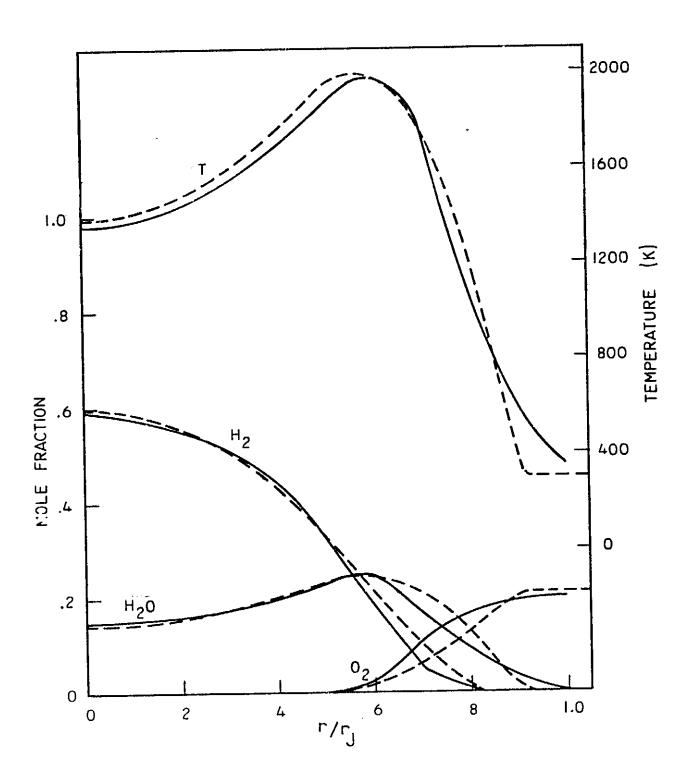
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